

Opposita-4(15),11-dien-1-«beta»-ol

Inchi:	InChI=1S/C15H24O/c1-10(2)9-12-7-8-15(4)13(16)6-5-11(3)14(12)15/h12-14,16H,1,3,5-9
InchiKey:	HLVNRJLLBUWVCO-OOJKYFRXSA-N
Formula:	C15H24O
SMILES:	<chem>C=C(C)CC1CCC2(C)C(O)CCC(=C)C12</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	135.26	kJ/mol	Joback Method
hf	-203.60	kJ/mol	Joback Method
hfus	20.76	kJ/mol	Joback Method
hvap	63.80	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mvol	197.760	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	647.69	K	Joback Method
tc	848.84	K	Joback Method
tf	358.33	K	Joback Method
vc	0.747	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.56	J/mol×K	647.69	Joback Method
cpg	589.28	J/mol×K	681.22	Joback Method
cpg	607.05	J/mol×K	714.74	Joback Method
cpg	623.99	J/mol×K	748.27	Joback Method
cpg	640.23	J/mol×K	781.79	Joback Method
cpg	655.87	J/mol×K	815.32	Joback Method
cpg	671.03	J/mol×K	848.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201279&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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